Attention

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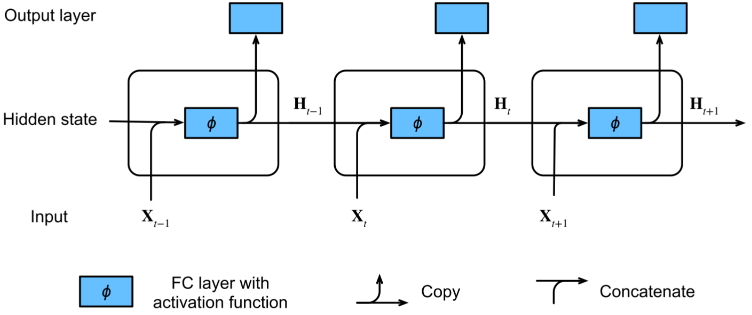
Outline

RNN



$$H_t = \phi\big(X_t W_{xh} + H_{t-1} W_{hh} + b_h\big)$$
$$O_t = H_t W_{hq} + b_q$$

$$X_t \in \mathbb{R}^{n\times d} \quad H_t \in \mathbb{R}^{n\times h}$$
$$O_t \in \mathbb{R}^{n\times q} \quad b_h \in \mathbb{R}^{1\times h}$$

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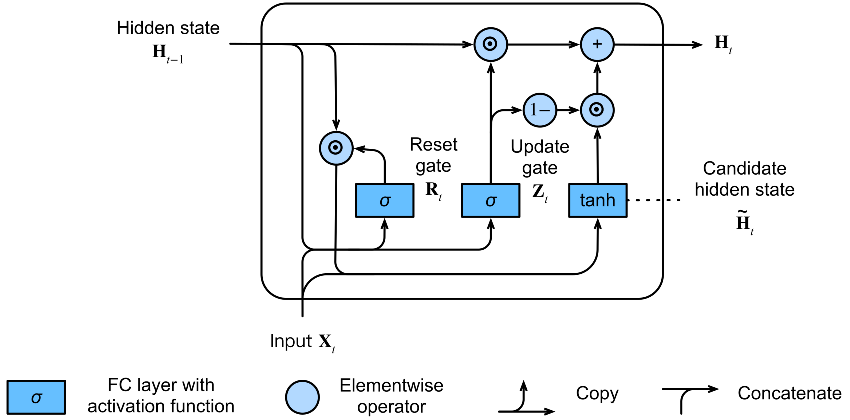
[1] Aston Zhang et al. "Dive into Deep Learning". In: *CoRR* abs/2106.11342 (2021). arXiv: 2106.11342. URL: https://arxiv.org/abs/2106.11342.

GRU Gated Recurrent Unit



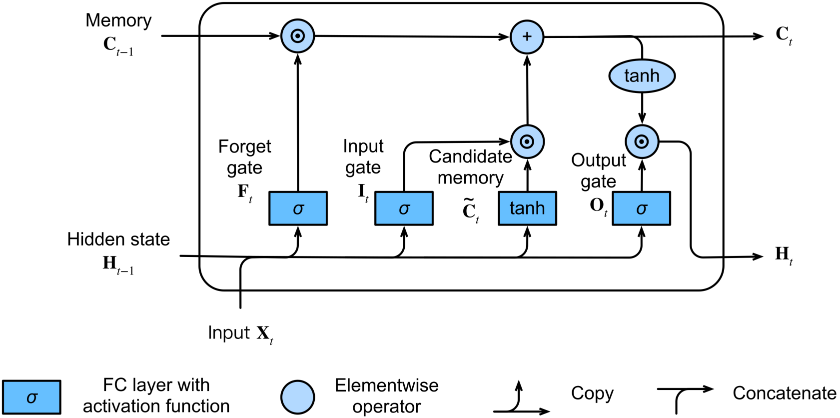
GRU Gated Recurrent Unit

GRU supports gating of the hidden state.

- Reset gates help capture short-term dependencies in sequences.
- Update gates help capture long-term dependencies in sequences.

$$
\begin{aligned}
R_t &= \sigma\left(X_t W_{xr} + H_{t-1} W_{hr} + b_r\right) \\
Z_t &= \sigma\left(X_t W_{xz} + H_{t-1} W_{hz} + b_z\right) \\
\tilde{H}_t &= \tanh\left(X_t W_{xh} + \left(R_t \odot H_{t-1}\right) W_{hh} + b_h\right) \\
H_t &= Z_t \odot H_{t-1} + \left(1 - Z_t\right) \odot \tilde{H}_t
\end{aligned}
$$

LSTM



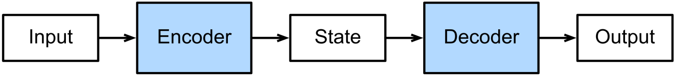
Memory
$\mathbf{C}_{t-1}$
$\mathbf{C}_t$
tanh
Forget gate
$\mathbf{F}_t$
σ
Input gate
$\mathbf{I}_t$
σ
Candidate memory
$\tilde{\mathbf{C}}_t$
tanh
Output gate
$\mathbf{O}_t$
σ
Hidden state
$\mathbf{H}_{t-1}$
$\mathbf{H}_t$
Input $\mathbf{X}_t$
σ
FC layer with activation function
Elementwise operator
Copy
Concatenate

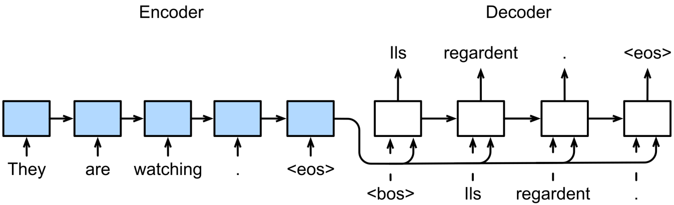
LSTM

The idea is similar to GRU.

$$
\begin{aligned}
I_t &= \sigma\big(X_t W_{xi} + H_{t-1} W_{hi} + b_i\big) \\
F_t &= \sigma\big(X_t W_{xf} + H_{t-1} W_{hf} + b_f\big) \\
O_t &= \sigma\big(X_t W_{xo} + H_{t-1} W_{ho} + b_o\big) \\
\tilde{C}_t &= \tanh\big(X_t W_{xc} + H_{t-1} W_{hc} + b_c\big) \\
C_t &= F_t \odot C_{t-1} + I_t \odot \tilde{C}_t \\
H_t &= O_t \odot \tanh(C_t)
\end{aligned}
$$

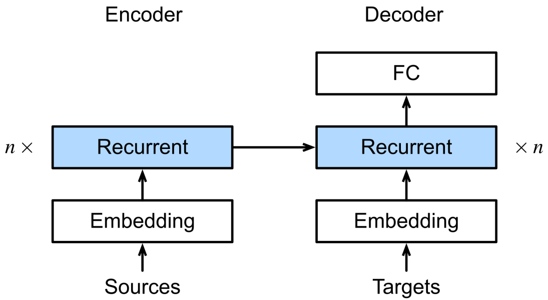
Encoder-Decoder





Encoder-Decoder

- Encoder: $H_t = f\big(X_t, H_{t-1}\big),\ C = g\big(H_1, \ldots, H_t\big)$
- Decoder: to get $P(Y_t | Y_1, \ldots, Y_{t-1}, C),\ H_t = g\big(Y_{t-1}, C, H_{t-1}\big)$.



Outline

Attention Prompt

A simple regression Problem: $f \in \{(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)\}$.

- Average Pooling:

$$f(x) = \frac{1}{n}\sum_{i=1}^{n} y_i$$

- Attention Pooling:

$$f(x) = \sum_{i=1}^{n} \alpha(x, x_i) y_i$$

We call x a *query* and (x_i, y_i) a *key-value* pair.
α is the attention weight, which is the target.[2]

[2] Aston Zhang et al. "Dive into Deep Learning". In: *CoRR* abs/2106.11342 (2021). arXiv: 2106.11342. URL: https://arxiv.org/abs/2106.11342.

Attention Prompt

- Nonparametric:

$$\alpha(x, x_i) = \frac{K(x - x_i)}{\sum_j K(x - x_j)}$$

$$K(u) = \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{u^2}{2}\right)$$

- parametric: learnable *Attention Scoring Function*

Outline

Transformer

- Relys entirely on multi-head self-attention
- Encoder-Decoder architecture
- Positional encoding

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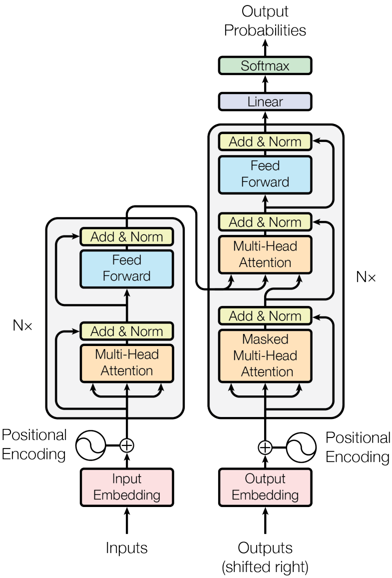
[3] Ashish Vaswani et al. "Attention Is All You Need". In: *CoRR* abs/1706.03762 (2017). arXiv: 1706.03762. URL: http://arxiv.org/abs/1706.03762.

Architecture



Encoder:

- $N = 6$ layers
- Multi-head self-attention $+$ feed forward

Decoder:

- Masked Multi-head self-attention
- Multi-head attention

Others:

- Positional Encoding
- Layer-normalization

Scoring Function

Scaled Dot-Product Attention

$$Attention(Q, K, V) = \mathsf{softmax}\left(\frac{QK^T}{\sqrt{d_k}}\right)V$$

$$Q \in \mathbb{R}^{n \times d_k} \quad K \in \mathbb{R}^{m \times d_k} \quad V \in \mathbb{R}^{m \times d_v}$$

Multi-Head Attention

It is beneficial to linearly project Q, K, V to d_k, d_k, d_v dimensions h times.

$$Multihead(Q, K, V) = Concat(head_1, \ldots, head_n)\,W^O$$
$$\text{where } head_i = Attention(QW_i^Q, KW_i^K, VW_i^V)$$

Self-attention:

$$\{f(x_i), 1 \leq i \leq n\}$$
$$\text{where } f \in \{(x_i, x_i)\}$$

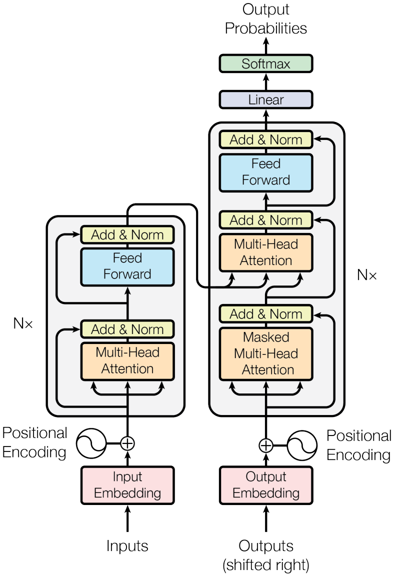
Positional Encoding

For $P \in \mathbb{R}^{n \times d}$:

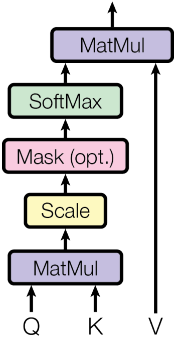
$$p_{pos,2i} = \sin\left(\frac{i}{10000^{2i/d}}\right)$$
$$p_{pos,2i+1} = \cos\left(\frac{i}{10000^{2i/d}}\right)$$

n length of sequence; d length of encoding.
Give each position-embedding pair a *unique* value.

Recap



Output Probabilities
Softmax
Linear
Add & Norm
Feed Forward
Add & Norm
Multi-Head Attention
Add & Norm
Masked Multi-Head Attention
Nx
Add & Norm
Feed Forward
Add & Norm
Multi-Head Attention
Nx
Positional Encoding
Positional Encoding
Input Embedding
Output Embedding
Inputs
Outputs (shifted right)

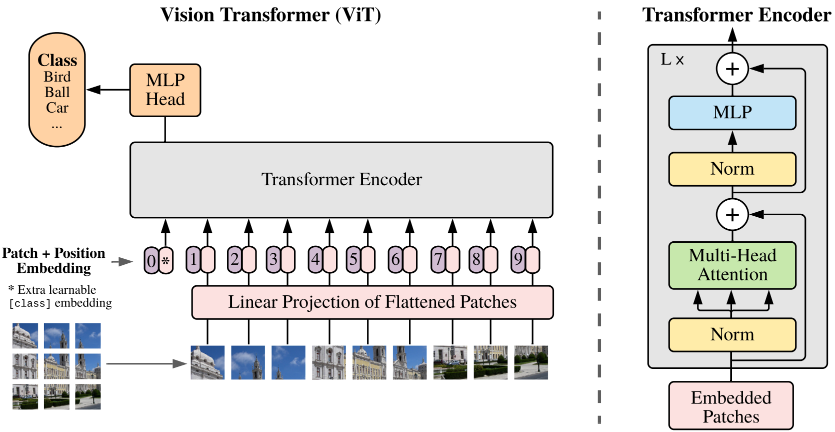


MatMul
SoftMax
Mask (opt.)
Scale
MatMul
Q
K
V

Outline

VIT Vision Transformer

Split images into fixed-size patches

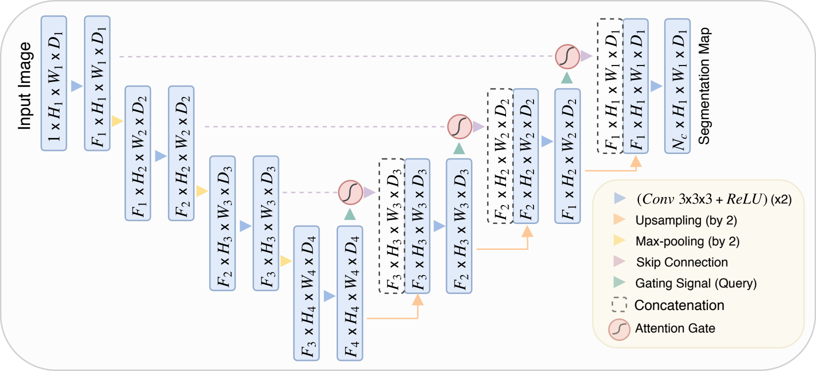


[4]

[4] Alexey Dosovitskiy et al. "An Image is Worth 16x16 Words: Transformers for Image Recognition at Scale". In: *CoRR* abs/2010.11929 (2020). arXiv: 2010.11929. URL: https://arxiv.org/abs/2010.11929.

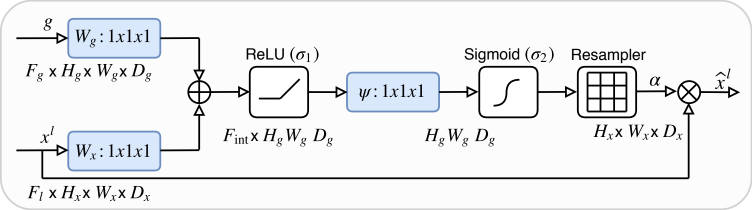
Outline

Attention UNet



$$Concat(Attention, upsample)$$

Attention Unet



Using *query* g from a coarser scale. Resampler Trilinear interpolation is applied.[5]

[5] Ozan Oktay et al. "Attention U-Net: Learning Where to Look for the Pancreas". In: *CoRR* abs/1804.03999 (2018). arXiv: 1804.03999. URL: http://arxiv.org/abs/1804.03999.

Outline

Inductive Bias

Component	Entities	Relations	Rel. inductive bias	Invariance
Fully connected	Units	All-to-all	Weak	-
Convolutional	Grid elements	Local	Locality	Spatial translation
Recurrent	Timesteps	Sequential	Sequentiality	Time translation
Graph network	Nodes	Edges	Arbitrary	Node, edge permutations

Peter W. Battaglia et al. "Relational inductive biases, deep learning, and graph networks". In: *CoRR* abs/1806.01261 (2018). arXiv: 1806.01261. URL: http://arxiv.org/abs/1806.01261

[1] Peter W. Battaglia et al. "Relational inductive biases, deep learning, and graph networks". In: *CoRR* abs/1806.01261 (2018). arXiv: 1806.01261. URL: http://arxiv.org/abs/1806.01261.

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[3] Ozan Oktay et al. "Attention U-Net: Learning Where to Look for the Pancreas". In: *CoRR* abs/1804.03999 (2018). arXiv: 1804.03999. URL: http://arxiv.org/abs/1804.03999.

[4] Ashish Vaswani et al. "Attention Is All You Need". In: *CoRR* abs/1706.03762 (2017). arXiv: 1706.03762. URL: http://arxiv.org/abs/1706.03762.

[5] Aston Zhang et al. "Dive into Deep Learning". In: *CoRR* abs/2106.11342 (2021). arXiv: 2106.11342. URL: https://arxiv.org/abs/2106.11342.